

1,5-Heptadiene, 7,7-difluoro-, (E)-

Inchi:	InChI=1S/C7H10F2/c1-2-3-4-5-6-7(8)9/h2,5-7H,1,3-4H2/b6-5+
InchiKey:	MIJUABDAXIPPLR-AATRIKPKSA-N
Formula:	C7H10F2
SMILES:	C=CCCC=CC(F)F
Mol. weight [g/mol]:	132.15
CAS:	85685-20-7

Physical Properties

Property code	Value	Unit	Source
gf	-215.94	kJ/mol	Joback Method
hf	-342.66	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	28.44	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.774		Crippen Method
mcvol	104.430	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
tb	358.50	K	Joback Method
tc	519.57	K	Joback Method
tf	147.99	K	Joback Method
vc	0.418	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.77	J/mol×K	358.50	Joback Method
cpg	193.18	J/mol×K	385.34	Joback Method
cpg	203.12	J/mol×K	412.19	Joback Method
cpg	212.60	J/mol×K	439.03	Joback Method
cpg	221.64	J/mol×K	465.88	Joback Method
cpg	230.26	J/mol×K	492.72	Joback Method
cpg	238.47	J/mol×K	519.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85685207&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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